Potential Energy Maps

Q.1) What are Potential Energy maps?

- **Potential Energy maps refer to the structural arrangement of atoms or molecules, maybe a result of chemical bonds due to interactions.**
- **It has a potential energy surface that describes the energy of a system, collection of atoms and terms of certain parameters normally the position of atoms.**
- **The surface might define energy as a function of one or more coordinates.**
- **It can be used to theoretically explore the properties of structure composed of atoms, for eg: finding the minimum energy shape of a molecule or computing rate of a chemical reaction.**
- **There are also Electrostatic Potential maps that illustrate the charge distribution of a 3d molecule. It allows us to visualize the variably charged regions of a molecule.**
- **EPM is fundamentally a measure of strength of nearby changes, nuclei and electrons at a particular position.**
- **To accurately analyze the charge distance of a molecule, a very large quantity of EPE values must be calculated.**
- **A computer program imposes the calculated data onto an electron density model of a molecule derived from Schrodinger equation.**

Q.2) Importance of Potential Energy maps.

- **Knowledge of the charge distribution can be used to determine how molecules interact with one another.**
- **Maps are invaluable in predicting the behavior of complex molecules.**
- **In creating an Electrostatic Potential energy map, important is to collect a very specific type of data, i.e., electrostatic potential surface.**
- **Advanced computer program calculates electrostatic potential energy at a set distant from the nuclei of the molecule.**

Q.3) How to locate and interpret EPE data?

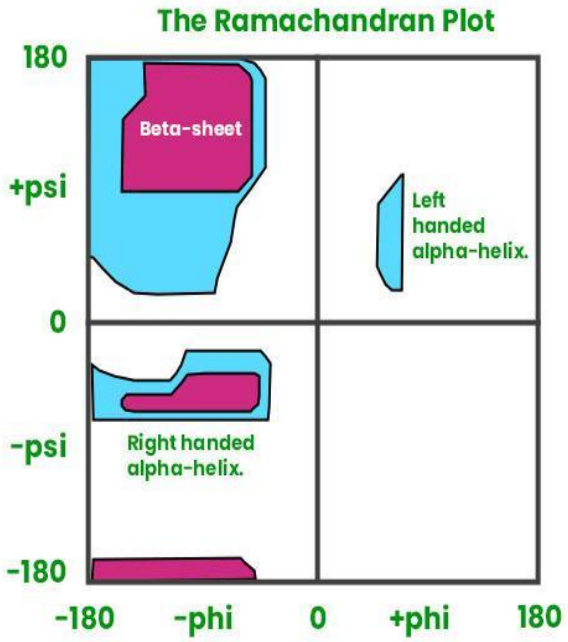
- **To make EPE data easy to interpret, color spectrum with RED as the lowest EPE value and BLUE as the highest EPE value, employed to convey varying intensities of the EPE values.**
- **To locate negatively and positively charged Electrostatic potential in molecules, Red indicates extreme negative and Blue indicates extreme positive.**

- **Red indicates minimum electrostatic potential, loosely bound or excess electrons and acts as an electrophilic attack.**
- **Blue indicates maximum electrostatic potential, tightly bound or less electrons and acts as a nucleophilic attack.**
- **To see all MEP surfaces, plot each surface as a contour around the molecule.**
- **Outer contour curves around the lower iso-surfaces and inner contour around higher iso-surface values.**
- **Surface is to indicate the available unoccupied space where excitation is going to reside around the molecule.**

Ramachandran Plot

Q.1)What is the RC plot? Explain in detail.

- **It is used for validating the structures.**
- **It includes two torsion angles of the polypeptide chain which describe the rotation of the polypeptide backbone around the bonds between N-C alpha called (Phi) and C alpha-C called (Psi).**
- **It provides an easy way to view the distribution of torsion angles of a protein structure.**
- **It provides an overview of the allowed and disallowed regions of torsion angle values; serves as an important indicator of quality of 3d protein structures.**
- **Let us consider an example of a RC plot showing four regions with blue, white and pink areas.**



- **White areas correspond to conformations where atoms in a polypeptide come closer than sum of their Vander Waals radii.**
- **Regions are sterically disallowed for all amino acids except glycine which is unique that it lacks a side chain.**
- **Pink regions correspond to conformations where there are no steric clashes, i.e, allowed regions.**
- **Blue areas show allowed regions if slightly shorter Vander Waals radii are used in calculation, i.e, atoms are allowed to come closer together bringing out additional region which corresponds to the left-handed alpha helix.**

Q.2)What are torsion angles?

- **Torsion angles are dihedral angles defined by four points in space.**
- **Two torsion angles Phi and Psi describe the rotation of the polypeptide chain around two bonds on both sides of C-alpha atom.**
- **Standard IUPAC definition of a dihedral angle illustrates the position of four atoms where rotation takes place around the central B-C bond.**
- **Positive bonds correspond to clockwise rotation.**
- **Protein backbone can be described with Phi, Psi and Omega as; PHI is the angle around -N-CA- bond with CA being alpha carbon, PSI is the angle around -CA-C- bond**

and OMEGA is the angle around -C-N- bond which is a peptide bond.

- **Torsion angles are among the most important local structural parameters that control protein folding.**
- **Third possible torsion angle with protein backbone is called Omega.**
- **They are able to predict 3d folding.**
- **Also provide flexibility required for the polypeptide backbone to adopt a certain fold, since omega is essentially flat and fixed to 180 degrees; due to partial double bond character of peptide bond that restricts rotation around the C-N bond, placing two successive alpha-carbons and C,O,N and H between them in one plane.**
- **Thus, rotation of protein chains can be described as rotation of peptide bond planes relative to each other.**
- **In a polypeptide, main chain of Phi and Psi angles are free to rotate.**
- **G N Ramachandran used computer models of small polypeptides to systematically vary Phi and Psi with the objective of finding stable conformations.**
- **Atoms are treated as hard spheres with dimensions corresponding to their Vander Waals radii.**
- **Therefore, Phi and Psi angles which cause spheres to collide correspond to sterically disallowed conformations of polypeptide backbone.**